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G-SFED model: Prediction of solvent effects on biological system for drug discovery

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Since most chemical and biochemical phenomena take place in solvent,the accurate and effective description of solvent effects on molecular structure, energy, and properties is very important in drug discovery. The solvation free energy of a solute is a fundamental quantity that represents the effect of solvation. Continuum solvent approach, an appealing alternative to explicit solvent approach, does not provide atomic resolution of individual solvent molecules, but it significantly improves the computational speed and reduces errors in statistical averaging that arise from incomplete sampling of solvent conformations. The generalized solvation free energy density (G-SFED) model, an advanced version of the SFED model proposed by No et al., is developed to compute the solvation free energies of a solute in any solvents. The solvation free energy of a solute is represented as a linear combination of empirical functions of the solute properties, and solvent effects on solvation were reflected in the linear expansion coefficients with a few solvent properties. Training and validation of the model were performed usingthe largest set of solvation free energies and provides a very fast and accurate generalized framework without complicated description of a solution. G-SFED has been applied to predict partition coefficients of small molecules and peptides, and to develop the 3D descriptors for prediction of interactions between protein and ligand.